

# Geometrical mutual information at the tricritical point of the two-dimensional Blume–Capel model

Ipsita Mandal,<sup>1</sup> Stephen Inglis,<sup>2</sup> and Roger G. Melko<sup>1,3</sup>

<sup>1</sup>*Perimeter Institute for Theoretical Physics, Waterloo, Ontario N2L 2Y5, Canada*

<sup>2</sup>*Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, D-80333 München, Germany*

<sup>3</sup>*Department of Physics and Astronomy, University of Waterloo, Ontario, N2L 3G1, Canada*

(Dated: July 18, 2016)

The spin-1 classical Blume–Capel model on a square lattice is known to exhibit a finite-temperature phase transition described by the tricritical Ising CFT in 1+1 space-time dimensions. This phase transition can be accessed with classical Monte Carlo simulations, which, via a replica-trick calculation, can be used to study the shape-dependence of the classical Rényi entropies for a torus divided into two cylinders. From the second Rényi entropy, we calculate the Geometrical Mutual Information (GMI) introduced by Stéphan *et. al.* [Phys. Rev. Lett. 112, 127204 (2014)] and use it to extract a numerical estimate for the value of the central charge near the tricritical point. By comparing to the known CFT result,  $c = 7/10$ , we demonstrate how this type of GMI calculation can be used to estimate the position of the tricritical point in the phase diagram.

*Introduction* – It is now well-established that there is a deep connection between certain measurable thermodynamic quantities and principles of information theory. Most straightforwardly, information can be quantified in terms of entropy, which can be defined from thermodynamic observables [1, 2]. For finite-temperature phase transitions, critical points are characterized by infinite correlation lengths, indicative of the existence of long-range channels for information transfer. It is interesting to ask whether observables derived from information quantities can be used to characterize classical phase transitions. Despite the answer being non-trivial, the Rényi entropies have recently been used to detect and classify phase transitions in a number of classical systems [3–10]. In particular, a mutual information derived from the second Rényi entropy [11–13] has been very successful in detecting finite-temperature critical points, even identifying their universality class without any *a priori* knowledge of an order parameter or associated broken symmetry.

The utility of the second Rényi entropy was demonstrated in a striking way by the introduction of the “Geometrical Mutual Information” (GMI) by Stéphan *et. al.* [4], where it was shown that a simple-to-implement classical Monte Carlo simulation of an Ising model at its phase transition was capable of calculating the central charge  $c$  of the associated 1+1-dimensional conformal field theory (CFT) [2, 14–17]. Most straightforwardly, if the simulation is tuned to twice the critical temperature  $T_c$  (for the second Rényi entropy), then a simple finite-size scaling analysis is sufficient to extract  $c$  using the functional form for the GMI obtained in Ref. [4] for a general CFT. It follows that one may employ the GMI in the converse manner: knowing the expected theoretical value of the central charge  $c$ , the GMI can be used to estimate the parameters which lead to criticality in a model. This may be useful when two or more parameters must be

tuned to realize a phase transition, such as occurs in the case of the tricritical Ising transition, which is described by a minimal CFT with  $c = 0.7$  [14, 15].

The simplest classical model that realizes a tricritical Ising point is the spin-1 Blume–Capel model. The Hamiltonian of the model on a two-dimensional square lattice [18, 19] is given by

$$H = -J \sum_{\langle ij \rangle} S_i^z S_j^z + D \sum_i (S_i^z)^2, \quad (1)$$

where  $S_i^z = (\pm 1, 0)$  and  $\langle ij \rangle$  denotes nearest-neighbor sites. Below, we have set the energy scale  $J = 1$ . The model has been shown to exhibit a tricritical point described by tricritical Ising CFT [20], though it cannot be solved exactly (non-integrable) away from criticality. The position of the tricritical point is non-universal and can only be determined numerically. There have been extensive studies in the literature using various sophisticated numerical techniques to pin down the values of the parameter  $D$  and temperature  $T$  of the tricritical point [21–35]. In this paper, we confirm through numerical calculation of the second Rényi entropy GMI that the central charge near the tricritical point is consistent with the value predicted by CFT,  $c = 7/10$ . In addition, we demonstrate how *a priori* knowledge of this universal constant can be used in conjunction with the GMI to provide an estimate for the position of the phase transition, without any reliance on the order parameter of the system.

*Method* – Let us consider a classical spin system defined on a square lattice with Hamiltonian Eq. (1). We can partition the lattice into two regions,  $A$  and  $B$ , with the spin configurations within each subsystem labeled as  $i_A$  and  $i_B$  respectively. The probability of state  $i_A$  occurring in subregion  $A$  is  $p_{i_A} = \sum_{i_B} p_{i_A, i_B}$ , where  $p_{i_A, i_B} = e^{-\beta E(i_A, i_B)} / Z[T]$  is the probability of existence

of any arbitrary state of the entire system, obtained from the Boltzmann distribution. Here  $E(i_A, i_B)$  is the energy associated with the states  $i_A$  and  $i_B$ ,  $\beta = 1/T$ , and  $Z[T] = \sum_{i_A, i_B} e^{-\beta E(i_A, i_B)}$  is the partition function of  $A \cup B$ .

Now the second Rényi entropy for subregion  $A$  is defined by [11]:

$$\begin{aligned} S_2(A) &= -\ln \left( \sum_{i_A} p_{i_A}^2 \right) \\ &= -\ln \left( \sum_{i_A} \frac{\sum_{i_B} e^{-\beta E(i_A, i_B)} \sum_{j_B} e^{-\beta E(i_A, j_B)}}{Z^2[T]} \right) \\ &= -\ln(Z[A, 2, T]) + 2 \ln(Z[T]), \end{aligned} \quad (2)$$

where  $Z[A, 2, T] = \sum_{i_A, i_B, j_B} e^{-\beta \{E(i_A, i_B) + E(i_A, j_B)\}}$  is the partition function of a new “replicated” system, such that the spins in subregion  $A$  are constrained to be the same in both the replicas, while the spins in subregion  $B$  are unrestricted for the two copies. The first condition leads the spins in the bulk of subregion  $A$  to behave as if their effective temperature is  $T/2$  for local interactions. The Rényi mutual information (RMI) can now be defined as the symmetric quantity:

$$\begin{aligned} I_2(A, B) &= S_2(A) + S_2(B) - S_2(A \cup B) \\ &= -\ln \left( \frac{Z[A, 2, T] Z[B, 2, T]}{Z^2[T] Z[T/2]} \right). \end{aligned} \quad (3)$$

This quantity has been demonstrated useful in the past for detecting finite-temperature phase transitions with great accuracy [3, 12, 13].

In two dimensions, the RMI can be used to define a universal quantity ( $\mathcal{G}_2$ ) called the geometric mutual information (GMI) [4],

$$I_2(A, B) = a_2 L + \mathcal{G}_2 + \mathcal{O}(1), \quad (4)$$

which is a function of the various aspect ratios in the system. Due to the symmetry of the RMI, all the bulk (“volume”) contributions occurring in the Rényi entropy cancel. This leaves the “area-law” as the leading order term in Eq. (4), proportional to  $L$ , which is the length of the boundary between the subregions  $A$  and  $B$ . In two dimensions, the exact expression for the partition function of a critical system can be found using CFT [4, 12, 36–45]. For free external boundary conditions at  $T = 2T_c$ , cutting an  $L_x \times L_y$  system into two rectangular subregions  $L_A \times L_y$  and  $L_B \times L_y$ , the expression for GMI is given by [4]:

$$\mathcal{G}_2 = \frac{c}{2} \ln \left( \frac{f(L_A/L_x) f(L_B/L_x)}{\sqrt{L_x} f(L_y/L_x)} \right). \quad (5)$$

Here,  $c$  is the central charge of the associated CFT description of the critical point appearing at temperature

$T_c$ , and  $f(u) = \eta(iu)$  (where  $\eta$  is the standard Dedekind eta function [46]). This allows us to define a finite-size scaling procedure to extract  $c$  from numerical calculations of the GMI.

We compute the GMI using Monte Carlo simulations and the transfer-matrix ratio trick for classical systems [47–49], using the formula

$$\begin{aligned} \frac{Z[A, 2, T]}{Z^2[T]} &= \prod_{i=0}^{N-1} \frac{Z[A_{i+1}, 2, T]}{Z[A_i, 2, T]}, \\ Z[A_0, 2, T] &= Z^2[T]. \end{aligned} \quad (6)$$

Here,  $A_i$  denotes a series of  $N$  blocks of increasing size, the consecutive blocks differing by a one-dimensional strip of spins running parallel to the boundary separating  $A$  and  $B$ , with  $A_0$  being the empty region and  $A_N = A$ . The algorithm is well documented in Ref. [4]. In addition to the procedure presented there, we combine parallel tempering to ensure that the states used to estimate the ratios of the partition functions,  $\left\{ \frac{Z[A_{i+1}, 2, T]}{Z[A_i, 2, T]} \right\}$ , are efficiently sampled. This is important when trying to accurately locate the tricritical point in the Blume-Capel model where critical slowing down can bias results from Monte Carlo simulations. In addition, having results over a grid of model parameters allows us to examine the quality of the fit to the universal shape function to compare to previous estimates for the tricritical temperature  $T_{tc}$  and the coupling constant  $D_{tc}$ .

For a square system at  $T = 2T_c$  and all other parameters corresponding to the critical point,  $c$  can be readily extracted from the quantity

$$I_2(\ell, L) - I_2(L/2, L) = \mathcal{J}(c) \equiv \frac{c}{2} \ln \left( \frac{f(\ell/L) f(1 - \ell/L)}{f^2(1/2)} \right). \quad (7)$$

We compute  $[I_2(\ell, L) - I_2(L/2, L)]$  numerically using Monte Carlo simulations at  $T = 2T_c$  and compared our data with this theoretical expectation. Of course, the numerical data thus obtained is affected by significant finite-size effects. Hence, in order to use the above expression to obtain  $c$ , we perform a finite-size extrapolation as described in the next section.

**Results** – We know that the Blume-Capel model has a line in the  $(D, T)$  plane representing a second-order (or continuous) phase transition, which terminates at the tricritical point, meeting another line corresponding to a first-order phase transition [50]. This line of phase transitions can be detected by the second Rényi entropy. As an example, Fig. 1 shows the RMI as a function of temperature for  $D = 1.965$ , revealing a transition at  $T_c$  and  $2T_c$  as crossings in  $I_2(L/2, L)/L$ . The data used for this plot has been obtained by thermodynamic integration and imposing periodic boundary conditions on the lattice. Although the RMI curve looks continuous, the fact that these parameters are inconsistent with the tricriti-

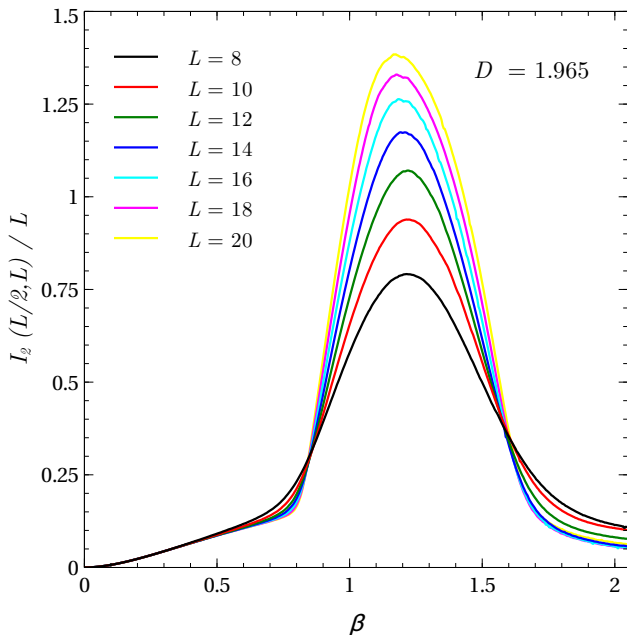


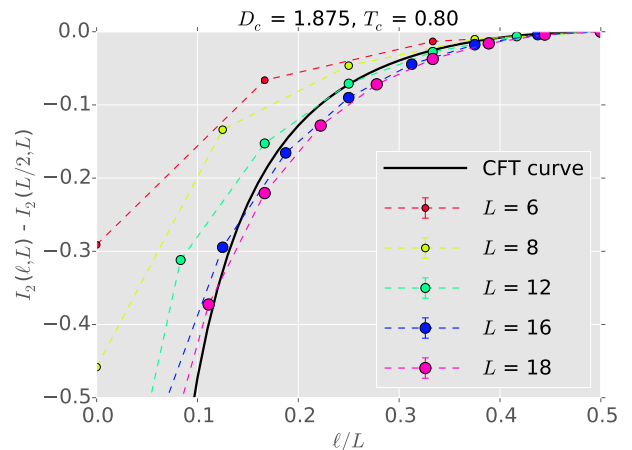
FIG. 1. (color online). The RMI per boundary length,  $I_2(L/2, L)/L$ , as a function of  $\beta$ . Crossings are seen at  $\beta_c/2$  and  $\beta_c$ .

cal point can be checked by calculating the central charge from GMI using a finite-size extrapolation.

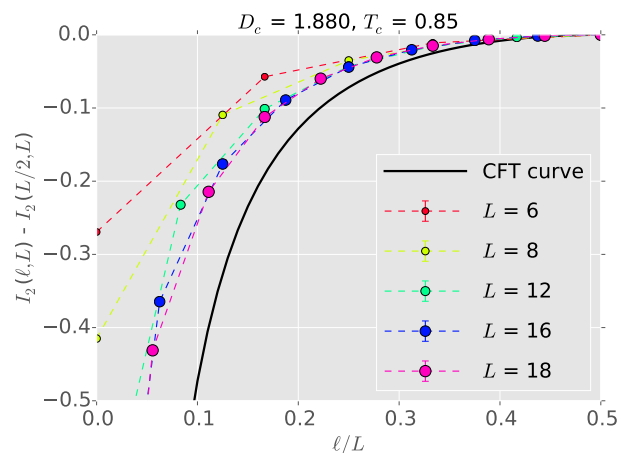
Let us elaborate on how this finite-size analysis can be implemented. The function  $y(1/L) = m/L + c_{\text{extr}}$  is obtained for each  $\ell/L$ , where  $m$  is the slope and  $c_{\text{extr}}$  is the  $y$ -intercept for the data points corresponding to  $(x \equiv 1/L, y(x) \equiv I_2(\ell, L) - I_2(L/2, L))$ . After collecting the  $\{c_{\text{extr}}\}$  for all ratios  $\{\ell/L\}$ , we fit these with the fitting function  $\mathcal{J}(c)$ , keeping  $c$  as the free parameter. In other words, the set  $\{\ell/L, c_{\text{extr}}\}$  is fitted by numerically searching for the value of  $c$  which makes  $\mathcal{J}(c)$  fit the data best. In addition, we have computed the  $\chi^2$  estimates, which tell us how close the numerically extracted values are to the theoretical prediction of  $c = 0.7$ .

For the Blume-Capel model, the GMI at the critical point depends on two parameters:  $D_c$  and  $T_c$ . This makes it harder to pin down the tricritical point compared to the models studied in earlier works by this same technique [3, 4], for which the critical point corresponding to a CFT were dependent only on the parameter  $T_c$ . We have scanned the parameter space to find the tricritical point. Fig. 2 shows the behavior of  $c$  as a function of the ratio  $\ell/L$ , for two sets of  $(D_c, T_c)$ , which do not give a central charge consistent with the theoretical tricritical value of 0.7, after fitting  $\{c_{\text{extr}}\}$  with  $\mathcal{J}(c)$ . This illustrates how we may discard values of  $(D, T)$  which have no possibility of corresponding to the tricritical point.

To obtain an estimate for the tricritical parameters  $T_{tc}$  and  $D_{tc}$ , we have implemented a two-step procedure as follows. In the first step, the best-fit  $c$



(a)

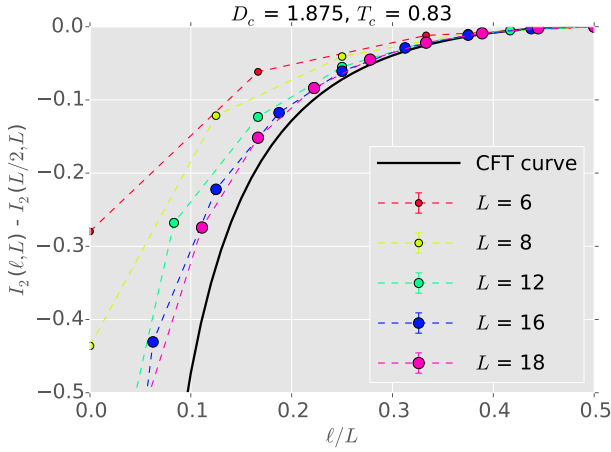


(b)

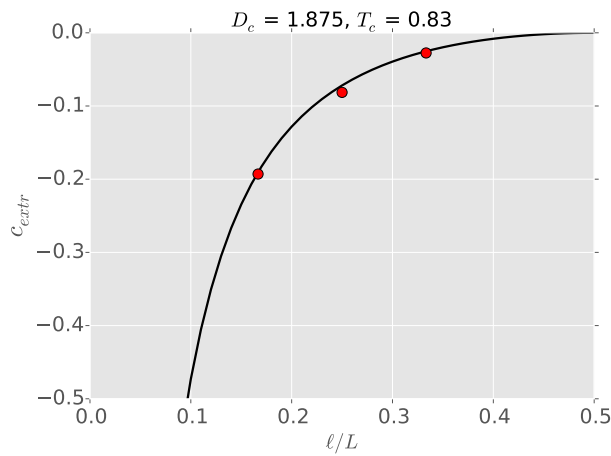
FIG. 2. (color online). Representative curves for values of  $(D_c, T_c)$  which are off-critical and hence do not give the central charge close to the theoretical value of 0.7 at the tricritical point. The “CFT curve” corresponds to the plot of  $\mathcal{J}(0.7)$ .

has been calculated from  $\{c_{\text{extr}}\}$ , as described above, for a range of sizes  $\{6, 8, 12, 16, 18\}$  and aspect ratios  $\{1/4, 1/6, 2/6, 1/8, 3/8\}$ . In the second step, we assume  $c$  is fixed to 0.7, and calculate a goodness-of-fit measure  $\chi^2$ . This  $\chi^2$ -estimate, which quantifies the quality of our fits to  $c = 0.7$ , is crucial in determining a region of critical parameters which gives our best-fit to the tricritical CFT form.

To obtain our estimate of the tricritical point, we have restricted our search to the region  $D_c \in \{1.735, 1.895\}$  and  $T_c \in \{0.80, 1.00\}$ , taking help from previous studies in the literature [28, 35], in order to make a judicious choice of the parameter ranges. Varying  $(D_c, T_c)$ , and repeating our finite-size extrapolation and  $\chi^2$  computation, we have found numerically that values consistent with  $c = 0.7$  are obtained roughly within this parameter



(a)



(b)

FIG. 3. (color online). The first plot shows the data points obtained for  $(D_c = 1.875, T_c = 0.83)$ , lying within the region of least  $\chi^2$ , with the “CFT curve” corresponding to  $\mathcal{J}(0.7)$ . The second plot shows that the points, obtained after finite-size extrapolation, lie on the CFT curve.

range. Fig. 3(a) shows  $[I_2(\ell, L) - I_2(L/2, L)]$  obtained for a representative point  $(D_c = 1.875, T_c = 0.83)$ , lying within the region of minimum  $\chi^2$ . Fig. 3(b) shows how well the  $\{c_{\text{extr}}\}$ , obtained from the finite-size extrapolation of this data set, fall on the expected CFT curve. This analysis can be summarized in the contour plot in Fig. 4, which illustrates the fitted values of  $c$ , together with an outline of the valley that occurs in the  $\chi^2$  measure for  $c = 0.7$ . The overlap gives us a range for our estimated value of  $T_{tc}$  and  $D_{tc}$ .

*Discussion* – In this paper, we have estimated the position of the tricritical point for the spin-1 classical Blume-Capel model on a square lattice by using classical Monte Carlo calculations of second Rényi entropy. First, by analyzing the Geometrical Mutual Information (GMI),

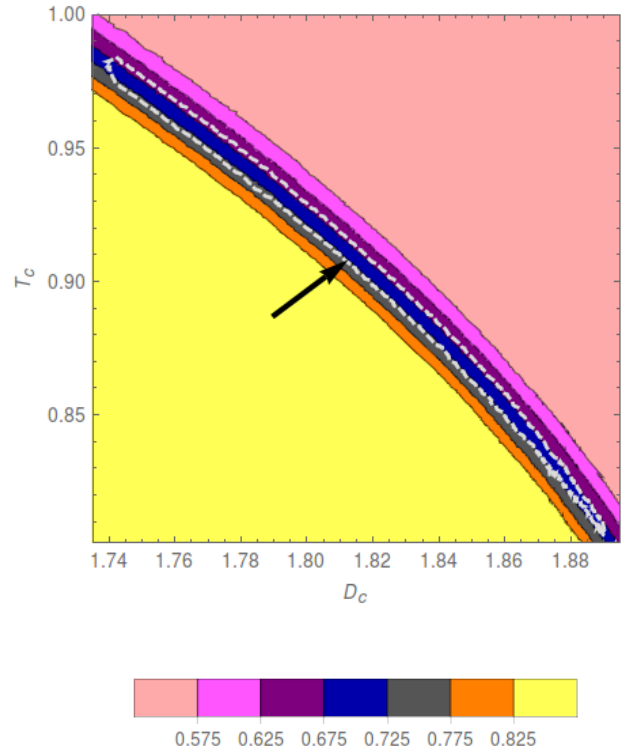


FIG. 4. (color online). The contourplot shows the  $c$ -contours in the  $(D_c, T_c)$ -plane, obtained by fitting the data to the universal shape function  $\mathcal{J}(c)$  after finite-size extrapolation. The region within  $D_c \in \{1.740, 1.895\}$  and  $T_c \in \{0.80, 0.97\}$  gives the closest match to the actual  $c = 0.7$ . The dashed silver line, highlighted by the arrow, encloses the region with least  $\chi^2$  (in arbitrary units), assuming fitting to  $c = 0.7$ .

we have calculated the central charge of the low-energy conformal field theory (CFT) description of the critical point, and confirmed that it agrees with the known theoretical value of  $c = 0.7$ . Then, restricting our range of model parameters by looking at the best-fit of the data to this value, we have obtained a range of coupling constants consistent with the tricritical point. Our technique is an interesting demonstration of the power of the GMI to distinguish tricritical CFTs numerically, without reliance on an order parameter or thermodynamic observable. However, determination of the Rényi entropy requires a calculation of a ratio of partition functions, which can only be obtained through thermodynamic integration, or variations of a “ratio-trick”. Thus, the system sizes obtained will be smaller than what is possible with conventional estimators. Attempting to control these finite-size effects with careful extrapolations leads to the conclusion that the tricritical point can be anywhere within the minimum  $\chi^2$  region of Fig. 4, lying in the range  $D_c \in \{1.735, 1.895\}$  and  $T_c \in \{0.80, 0.97\}$ . This region is consistent with the previous surveys in literature, obtained through a variety of other numerical techniques [35]. This shows that de-

spite difficulties related to limitations imposed by finite-size effects, it is relatively straightforward to obtain a reasonable estimate of the tricritical point from our Rényi entropy data.

For the model studied in this paper, where the central charge is known, we have demonstrated how its knowledge can be used to provide an estimate of two parameters ( $D_c, T_c$ ) which define the tricritical point. The same procedure could be applied in other interesting systems, where the order parameter is not known, but which contain critical lines with well-defined  $c$ -values [51]. In other higher-dimensional models, where the system cannot be mapped to  $(1+1)$ -dimensional CFTs, it would be interesting to extend the definition of the GMI to explore higher-dimensional analogues of  $c$ , if the values of critical parameters are known. This would further establish the diverse utility of information theory techniques in the arena of statistical mechanics and condensed-matter theory.

*Acknowledgments* – We thank P. Fendly for enlightening discussions. I.M. is grateful to A. Bhattacharya and L. E. Hayward Sierens for helping with the basics of coding. This work was made possible by the computing facilities of SHARCNET. Support was provided by NSERC of Canada (I.M. and R.G.M.), the Templeton Foundation (I.M.), the FP7/ERC Starting Grant No. 306897 (S.I.), and the National Science Foundation under Grant No. NSF PHY11-25915 (R.G.M). Research at the Perimeter Institute is supported, in part, by the Government of Canada through Industry Canada and by the Province of Ontario through the Ministry of Research and Information.

- 
- [1] C. E. Shannon, ACM SIGMOBILE Mobile Computing and Communications Review **5**, 3 (2001).
  - [2] P. Calabrese, J. Cardy, and B. Doyon, Journal of Physics A: Mathematical and Theoretical **42**, 500301 (2009).
  - [3] J. Iaconis, S. Inglis, A. B. Kallin, and R. G. Melko, Phys. Rev. B **87**, 195134 (2013).
  - [4] J.-M. Stéphan, S. Inglis, P. Fendley, and R. G. Melko, Phys. Rev. Lett. **112**, 127204 (2014).
  - [5] J. Wilms, M. Troyer, and F. Verstraete, Journal of Statistical Mechanics: Theory and Experiment **2011**, P10011 (2011).
  - [6] J. Wilms, J. Vidal, F. Verstraete, and S. Dusuel, Journal of Statistical Mechanics: Theory and Experiment **2012**, P01023 (2012).
  - [7] V. Alba, Journal of Statistical Mechanics: Theory and Experiment **2013**, P05013 (2013).
  - [8] C.-M. Chung, V. Alba, L. Bonnes, P. Chen, and A. M. Läuchli, Phys. Rev. B **90**, 064401 (2014).
  - [9] V. Alba, S. Inglis, and L. Pollet, Phys. Rev. B **93**, 094404 (2016).
  - [10] J. Helmes, J.-M. Stéphan, and S. Trebst, Phys. Rev. B **92**, 125144 (2015).
  - [11] R. G. Melko, A. B. Kallin, and M. B. Hastings, Phys. Rev. B **82**, 100409 (2010).
  - [12] R. R. P. Singh, M. B. Hastings, A. B. Kallin, and R. G. Melko, Phys. Rev. Lett. **106**, 135701 (2011).
  - [13] S. Inglis and R. G. Melko, Phys. Rev. E **87**, 013306 (2013).
  - [14] A. Belavin, A. Polyakov, and A. Zamolodchikov, Nuclear Physics B **241**, 333 (1984).
  - [15] D. Friedan, Z. Qiu, and S. Shenker, Phys. Rev. Lett. **52**, 1575 (1984).
  - [16] C. Holzhey, F. Larsen, and F. Wilczek, Nuclear Physics B **424**, 443 (1994).
  - [17] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003).
  - [18] M. Blume, Phys. Rev. **141**, 517 (1966).
  - [19] H. Capel, Physics Letters **23**, 327 (1966).
  - [20] D. B. Balbao and J. R. D. de Felicio, Journal of Physics A: Mathematical and General **20**, L207 (1987).
  - [21] T. W. Burkhardt, Phys. Rev. B **14**, 1196 (1976).
  - [22] A. N. Berker and M. Wortis, Phys. Rev. B **14**, 4946 (1976).
  - [23] T. W. Burkhardt and H. J. F. Knops, Phys. Rev. B **15**, 1602 (1977).
  - [24] W. M. Ng and J. H. Barry, Phys. Rev. B **17**, 3675 (1978).
  - [25] A. K. Jain and D. P. Landau, Phys. Rev. B **22**, 445 (1980).
  - [26] W. Selke and J. Yeomans, Journal of Physics A: Mathematical and General **16**, 2789 (1983).
  - [27] K. G. Chakraborty, Phys. Rev. B **29**, 1454 (1984).
  - [28] P. D. Beale, Phys. Rev. B **33**, 1717 (1986).
  - [29] D. P. Landau and R. H. Swendsen, Phys. Rev. B **33**, 7700 (1986).
  - [30] J. Tucker, T. Balcerzak, M. Gzik, and A. Sukiennicki, Journal of Magnetism and Magnetic Materials **187**, 381 (1998).
  - [31] A. Du, Y. Y., and H. Liu, Physica A: Statistical Mechanics and its Applications **320**, 387 (2003).
  - [32] A. Du, H. J. Liu, and Y. Q. Y., physica status solidi (b) **241**, 175 (2004).
  - [33] J. A. Plascak, J. G. Moreira, and F. C. SáBarreto, Physics Letters A **173**, 360 (1993).
  - [34] C. J. Silva, A. A. Caparica, and J. A. Plascak, Phys. Rev. E **73**, 036702 (2006).
  - [35] Y. Yüksel, U. Akinci, and H. Polat, Physica Scripta **79**, 045009 (2009).
  - [36] P. Kleban and I. Vassileva, Journal of Physics A: Mathematical and General **24**, 3407 (1991).
  - [37] P. Kleban and I. Vassileva, Journal of Physics A: Mathematical and General **25**, 5779 (1992).
  - [38] R. Bondesan, J. L. Jacobsen, and H. Saleur, Nuclear Physics B **867**, 913 (2013).
  - [39] J. L. Cardy and I. Peschel, Nuclear Physics B **300**, 377 (1988).
  - [40] E. Fradkin and J. E. Moore, Phys. Rev. Lett. **97**, 050404 (2006).
  - [41] M. P. Zaletel, J. H. Bardarson, and J. E. Moore, Phys. Rev. Lett. **107**, 020402 (2011).
  - [42] J.-M. Stéphan, G. Misguich, and V. Pasquier, Phys. Rev. B **84**, 195128 (2011).
  - [43] E. Fradkin, *Field Theories of Condensed Matter Physics*, 2nd ed. (Cambridge University Press, 2013).
  - [44] H. W. J. Blöte, J. L. Cardy, and M. P. Nightingale, Phys. Rev. Lett. **56**, 742 (1986).
  - [45] I. Affleck, Phys. Rev. Lett. **56**, 746 (1986).
  - [46] M. Abramowitz and I. A. Stegun, eds., *Handbook of*

- Mathematical Functions with Formulas, Graphs and Mathematical Tables* (Dover Publications, Inc., New York, 1965).
- [47] A. Gelman and X.-L. Meng, *Statist. Sci.* **13**, 163 (1998).
  - [48] S. Humeniuk and T. Roscilde, *Phys. Rev. B* **86**, 235116 (2012).
  - [49] M. Molkaraie and H.-A. Loeliger, *ArXiv e-prints* (2013), arXiv:1307.3645 [cs.IT].
  - [50] These two lines, in spite of representing phase transitions of different orders, actually form one continuous line separating the ordered phase from the disordered (or paramagnetic) phase.
  - [51] N. Chepiga, I. Affleck, and F. Mila, *Phys. Rev. B* **93**, 241108 (2016).